QUARTERLY PROGRESS REPORT

Study of Recirculating Gas Flow Fields in the Base Region of Saturn-Class Vehicles

NASA Contract No. NAS 8-11485

submitted to

National Aeronautics and Space Administration
George C. Marshall Space Flight Center
Huntsville, Alabama
Attention: PR-EC

prepared by

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Reporting Period: May 1, 1966 - July 31, 1966

1. Introduction

The work performed at Purdue University, on contract NAS 8-11485 during the three month period ending on July 30, 1966, was directed to the statistics of band models. The purpose of this phase of the contract is to clarify the statistical basis of the current models, in order to be able to extend their validity to a broader range of temperatures and pressures. This work is in a very early stage; this report is essentially a review of the available material, mostly that of Plass.

2. Fundamental Statistical Basis for Modeling in Uniform Gases

Inspection of a diagram of line intensities versus frequency plainly suggests that the main feature of the diagram is the nearly random distribution of line intensities and positions. Although it is known that these are connected by quantum-mechanical formulas, it suggests that in practice it may be sufficient to consider a random model.

The statistical model of a band assumes that the position and intensity of a given spectral line can be specified only by probability functions. In the derivation of statistical band models the assumptions that the positions of the spectral lines occur at random within a given frequency interval and that there is no correlation between the positions of the various lines have been made. The spectral line positions are represented by independent random variables and the intensity is also represented by a probability distribution which is independent of the line position.

The starting point in the development of random band models is Beer's exponential law for spectral transmittance.

$$T_\nu = \exp(-k_\nu L) = \exp(-S\, b(\nu)\, L) \qquad (1)$$

where k_ν is the linear absorption coefficient in cm^{-1} and L is the path length of the absorbing gas in cm. k_ν can also be written in terms of S the line intensity, and $b(\nu)$ the line shape.

Let $N(\nu_1,\ldots \nu_n)\ d\nu_1,\ldots d\nu_n$ be the joint probability density function for line position. It is the probability that the center of the first line is in frequency interval $d\nu_1$ when the center of the second is in frequency interval $d\nu_2$ etc. up to line n. The origin for frequency is taken to be at the center of a frequency interval of length D. Furthermore the joint probability that the lines will also simultaneously have an intensity in interval dS_1, dS_2 is $P(S_1,\ldots S_n)\ dS_1 \ldots dS_n$. This is the probability that the first line has intensity in the interval dS_1 when the second is in intensity interval dS_2 etc. up to the n^{th} intensity.

Now the transmittance at frequency ν is equal to the probability that there is a line at ν times the probability that the line has an intensity times the expression on the right-hand side of Beer's Law. Consequently the average transmittance over the frequency interval D is the integral of the transmittance over D, which is written as

$$\bar{T} = \int_{-D/2}^{D/2} \cdots \int_{-D/2}^{D/2} N(\nu_1 \cdots \nu_n) \left[\int_0^{\infty} \cdots \int_0^{\infty} P(S_1 \cdots S_n) \exp(-S_1 b(\nu)L \ldots -S_n b(\nu)L) \right.$$

$$\left. dS_1 \cdots dS_n \right] d\nu_1 \cdots d\nu_n \qquad (2)$$

where it is understood that the probability distributions are normalized over their respective intervals. Eq. (2) is the general expression for transmittance from a band of width D.

If one assumes that the spectral intensities are independent and identically distributed, one has

$$P(S_1 \ldots S_n)\, dS_1 \ldots dS_n \longrightarrow P(S_1) \ldots P(S_n)\, dS_1 \ldots dS_n = \prod_{i=1}^{n} P(S_i)\, dS_i \qquad (3)$$

Now the average transmittance becomes

$$\bar{T} = \int_{-D/2}^{D/2} \cdots \int_{-D/2}^{D/2} N(\nu_1 \ldots \nu_n) \left[\int_0^{\infty} \cdots \int_0^{\infty} \prod_{i=1}^{n} \left(P(S_i) \exp(-S_i b(\nu) L)\, dS_i \right) \right] d\nu_1 \ldots d\nu_n \qquad (4)$$

If one now makes the very important and fundamental assumption that any one arrangement of the line positions is equally probably to any other arrangement the joint probability distribution, $N(\nu_1 \ldots \nu_n)$ becomes a constant and the average transmittance in the frequency interval D can be written as

$$\bar{T} = \frac{1}{C^n} \int_{-D/2}^{D/2} \cdots \int_{-D/2}^{D/2} \left\{ \int_0^{\infty} \cdots \int_0^{\infty} \prod_{i=1}^{n} P(S_i) \exp(-S_i b(\nu) L)\, dS_i \right\} d\nu_1 \ldots d\nu_n \qquad (5)$$

The constant C is due to normalization of the previous joint probability density function. It is usually assumed that each spectral line is distributed independently with a uniform probability distribution in the frequency interval D. Then the constant C is equal to D, the frequency interval length. In summary, one has now assumed that it is equally probable that each line has its center at a given frequency in the frequency

interval D regardless of the position of the other lines and that the intensities are independent of each other and the line positions. It is easily seen that integral over each line is equal to the integral over every other line, if each has the same line shape, $b(\nu)$, so

$$\bar{T} = \left\{ D^{-1} \int_{-D/2}^{D/2} \left[\int_0^\infty P(S) \exp(-S\, b(\nu) L)\, dS \right] d\nu \right\}^n \tag{6}$$

This may be rewritten as

$$\bar{T} = \left\{ 1 - D^{-1} \int_{-D/2}^{D/2} \left[\int_0^\infty P(S) \left[1 - \exp(-S\, b(\nu)\, L) \right] dS \right] d\nu \right\}^n \tag{7}$$

Now one notes that if the order of integration is changed the average transmittance, $\bar{T}$, will envolve the equivalent width of a single line $W_{SL,D}$, in the frequency interval D.

$$\bar{T} = \left\{ 1 - D^{-1} \int_0^\infty P(S) \left[\int_{-D/2}^{D/2} \left[1 - \exp(-S\, b(\nu) L) \right] d\nu \right] dS \right\}^n \tag{8}$$

where

$$W_{SL,D} = \int_{-D/2}^{D/2} \left[1 - \exp(-S\, b(\nu) L) \right] d\nu \tag{9}$$

Consequently one can write

$$\overline{T} = \left\{ 1 - \frac{1}{D} \int_0^\infty P(S)\, W_{SL,D}\,(S, \alpha)\, dS \right\}^n \tag{10}$$

where α is the line half-width. Since $D = n\,d$, where d is the average interval between each spectral line and the average absorption $\overline{A} = 1 - \overline{T}$ one can write

$$\overline{A} = 1 - \left\{ 1 - \frac{1}{n\,d} \int_0^\infty P(S)\, W_{SL,D}\,(S, \alpha)\, dS \right\}^n \tag{11}$$

If one lets the number of lines in the band, n, approach infinity while the average spacing, d, is kept constant the frequency interval becomes infinite. By expanding the expression one notices that in the limit as n approaches infinity the average absorptance becomes exponential

$$\overline{A} = 1 - \exp\left[- \frac{1}{d} \left\{ \int_0^\infty P(S)\, W_{SL}\, dS \right\} \right] \tag{12}$$

where W_{SL} is the equivalent width of a single line for an infinite frequency interval.

The general expression for absorption from a finite number and an infinite number of randomly spaced spectral lines is given respectively by Eqs. (11) and (12). These equations show that the absorption of a band including all effects of overlapping of the spectral lines can be obtained from two quantities, the equivalent width of a single line in the appropriate frequency interval and the probability distribution of the intensities. This occurs because of the assumption that the line positions are independent of ν. (See Eq. 5)

For a Lorentz line shape and an infinite frequency interval the equivalent width, W_{SL} is

$$W_{SL} = 2\pi\alpha x e^{-x} [I_0(x) + I_1(x)] \tag{13a}$$

where

$$x = SL/2\pi\alpha \tag{13b}$$

and $I_0(x)$ and $I_1(x)$ are Bessel functions of imaginary argument. Eqn. (13) is called the Landenberg-Reiche formula.

A statistical band model often used is the random Elsasser model. The Elsasser band is assumed to consist of an infinite number of spectral lines, each with the same intensity, S, and half width α, and all the lines are equally spaced by d units from their neighbors. An exact expression for absorption summed over the band was first found by Elsasser. The fractional absorption, A, integrated over the frequency range d for an Elsasser band is

$$A = 1 - \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{-[\beta x \sinh\beta/(\cosh\beta - \cos Z)]} dZ \tag{14a}$$

where

$$\beta = 2\pi\alpha/d \tag{14b}$$

and x is defined by Eqn. (13b).

At small values of x the absorption is entirely determined by the total strength of all the absorbing lines and the Elsasser and statistical models agree. As x increases the results calculated from the two models begin to diverge; the Elsasser theory always gives more absorption (less transmission). The reason for this is that there is always more overlapping of the spectral lines in the statistical model than with the regular arrangement of lines in the Elsasser model; thus for a given pressure and path length the total line strength is more efficiently used in the Elsasser model.

An actual band has its lines arranged neither completely at random nor completely regularly. The actual pattern is formed by the superposition of many systems of lines. Hence the absorption can be represented very accurately by the random Elsasser model. The random Elsasser is a generalization of the Elsasser and statistical models in that it assumes that the absorption can be represented by the random superposition of Elsasser bands. Each individual Elsasser band may have different line spacings, half-widths and intensities. As the number of superposed Elsasser bands becomes large the absorption approaches that of the usual statistical model.

Let Δ_i be the separation of the spectral lines in the i^{th} Elsasser band, and N the total number of superposed Elsasser bands. Then the average spacing, δ, between the spectral lines is

$$\delta = \left[\sum_{i=1}^{N} \frac{1}{\Delta_i} \right]^{-1} \tag{15}$$

The equivalent width, $W_{E,i}$ of the i^{th} Elsasser band is

$$W_{E,i}(x_i, \beta_{\Delta_i}) = \Delta_i A_{E,i}(x_i \beta_{\Delta_i}) \tag{16}$$

where $\beta_{\Delta_i} = 2\pi\alpha_i/\Delta_i$ and $A_{E,i}$ is given by Eqn. (14a). The line spacing, half width and intensity are in general different for each Elsasser band.

By the same argument as was used to derive Eqn. (5) the absorption from a random superposition of Elsasser bands is

$$A = 1 - \left[\prod_{i=1}^{N} \Delta_i\right]^{-1} \int_{-\Delta_1/2}^{\Delta_1/2} \cdots \int_{-\Delta_N/2}^{\Delta_N/2} \left[\int_0^\infty \cdots \int_0^\infty \prod_{i=1}^{N} P_E(S_i) \exp(-S_i b_i(\gamma_i) L) dS_i\right] d\gamma_1 \cdots d\gamma_N \tag{17}$$

Interchanging the order of integration and noting the definition of the equivalent width $W_{E,i}(x_i, \beta_{\Delta_i})$ one has

$$A = 1 - \prod_{i=1}^{N} \left[\int_0^\infty \left[1 - \frac{W_{E,i}(\beta_{\Delta_i}, x_i)}{\Delta_i}\right] P_E(S_i) dS_i\right] \tag{18}$$

This is the general result for the absorption from a random superposition of N Elsasser bands, each of which may have different line spacings, half widths and intensities.

When $N = 1$ the absorption given by Eqn. (18) is just that given by the Elsasser model. As N increases and the average line spacing δ is held constant the absorption given by Eqn. (18) approaches that given by the random band model. In order to easily show this it is assumed that Δ_i and α_i are the same for each Elsasser band. Then Eqn. (18) becomes

$$A = 1 - \left[1 - \frac{1}{N\delta} \int_0^\infty W_E P_E (S)\, dS\right]^N \tag{19}$$

where

$$\Delta = N\delta$$

As N approaches infinity for fixed δ, Δ also approaches infinity and β, $(2\pi\alpha/\Delta)$, approaches zero. But for any finite value of x, $(SL/2\pi\alpha)$, as β approaches zero, there is no longer any effect of overlapping in a single Elsasser band as the spectral lines in the single band become separated by large frequency intervals, Δ. Thus in the limit Eqn. (19) and Eqn. (11) are identical, and the absorption is given by Eqn. (12) which is the expanded version of Eqn. (11). Thus it is seen that the random Elsasser band model provides a smooth transition between the absorption curves for the limiting cases of the Elsasser and Statistical models. The usual statistical model can, hence, be considered to be the superposition of a large number of Elsasser bands.

3. References

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4. Work Planned for the Next Quarterly Period

The work described herein on the evaluation of statistical radiation band models will be continued. In addition, work on chemical effects in the base flow region will be resumed. Specifically, an attempt will be made to evolve a simplified reaction model for the complex reaction system associated with plume afterburning. Also, the mechanisms of carbon formation will be reviewed to try to explain the magnitudes of solid carbon particles found in gas generator and main engine exhausts.